

Supporting Information for

La₆Cd_{0.75}Ga₂Q_{11.5}Cl_{2.5} (Q = S and Se): Two New Nonlinear Optical Chalcogenides with Large Laser- Induced Damage Threshold (LIDT)

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Supporting Tables and Figures

Table S1. Crystallographic Data and Experimental Details.

Formula	$\text{La}_6\text{Cd}_{0.75}\text{Ga}_2\text{S}_{11.5}\text{Cl}_{2.5}$	$\text{La}_6\text{Cd}_{0.75}\text{Ga}_2\text{S}_{11.5}\text{Cl}_{2.5}$
Formula weight	1514.46	2053.81
Temperature (K)	300	300
Wavelength (Å)	0.71073	0.71073
Crystal system	Hexagonal	Hexagonal
Space group	$P6_3$	$P6_3$
Unit cell dimensions (Å)	$a=b=10.1788(3)$ $c=6.0633(2)$	$a=b=10.4394(3)$ $c=6.4132(2)$
Volume (Å ³)	544.0(4)	605.2(8)
$\rho_{\text{(calc.)}}$ (g/cm ³)	4.621	5.65
Z	1	1
$F(000)$	666	876
Theta range for data collection(°)	2.31 to 30.47	2.25 to 25.16
Crystal size (mm)	0.04×0.03×0.025	0.05×0.03×0.03
Limiting indices	$-14 \leq h \leq 14, -14 \leq k \leq 13,$ $-8 \leq l \leq 8$	$-12 \leq h \leq 12, -12 \leq k \leq 12,$ $-7 \leq l \leq 6$
Independent refl.	$R_{\text{int}}=0.033$	$R_{\text{int}}=0.030$
Completeness to	100%	100%
Goodness-of-fit	1.121	1.168
R indices [all data]	$R_1=0.0182$ $wR_2=0.0352$	$R_1=0.0200$ $wR_2=0.0459$
Final R indices [$>2\sigma(I)$]	$R_1=0.0165$ $wR_2=0.0348$	$R_1=0.0194$ $wR_2=0.0458$
Extinction coeff.	0.009557	0.003153

Largest diff. peak and hole ($e \cdot \text{\AA}^{-3}$)	0.945 and -1.176	1.296 and -1.142
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Table S2. Atomic coordinates equivalent isotropic displacement parameters for



Atoms	<i>Wyck.</i>	<i>x</i>	<i>y</i>	<i>z</i>	S.O.F.	U_{eq} (\AA^2)
La1	6 <i>c</i>	0.7683(2)	0.1419(0)	0.8911(1)	1	0.017(3)
Cd1	2 <i>a</i>	0	0	0.6457(1)	0.373	0.060(5)
Ga1	2 <i>b</i>	2/3	1/3	0.4708(9)	0.875	0.011(7)
Ga2	6 <i>c</i>	0.7203(1)	0.2498(1)	0.4182(0)	0.042	0.011(7)
S1	2 <i>b</i>	2/3	1/3	0.1025(4)	1	0.011(6)
S2	6 <i>c</i>	0.5190(3)	0.0968(5)	0.6202(2)	0.875	0.014(8)
Cl2	6 <i>c</i>	0.5190(3)	0.0968(5)	0.6202(2)	0.125	0.014(8)
S3	6 <i>c</i>	0.7507(9)	-0.1527(5)	0.8563(4)	0.78	0.025(8)
Cl3	6 <i>c</i>	0.7507(9)	-0.1527(5)	0.8563(4)	0.22	0.025(8)

Table S3. Selected bond length $\text{La}_6\text{Cd}_{0.75}\text{Ga}_2\text{S}_{11.5}\text{Cl}_{2.5}$

Bond	Bond lengths (\AA)	Bond	Bond lengths (\AA)
La1-S1	2.9201	Cd1-S3	2.5573
La1-S2	2.8606	Ga1-S1	2.2342
La1-S2	2.9672	Ga1-S2	2.2924
La1-S2	3.0469	Ga2-S1	2.2671
La1-S3	2.9217	Ga2-S2	2.1881
La1-S3	2.9572	Ga2-S2	2.2221
La1-S3	3.0310	Ga2-S3	2.5021

Table S4. Atomic coordinates equivalent isotropic displacement parameters for

Atoms	<i>Wyck.</i>	<i>x</i>	<i>y</i>	<i>z</i>	S.O.F.	U_{eq} (Å ²)
La1	6 <i>c</i>	0.2193(5)	0.8461(4)	0.1065(8)	1	0.025(5)
Cd1	2 <i>a</i>	0	0	0.3486(1)	0.376	0.057(2)
Ga1	2 <i>b</i>	1/3	2/3	0.5240(4)	0.883	0.018(3)
Ga2	6 <i>c</i>	0.7203(1)	0.2498(1)	0.4182(0)	0.039	0.018(3)
Se1	2 <i>b</i>	1/3	2/3	0.8930(3)	1	0.015(5)
Se2	6 <i>c</i>	0.4777(3)	0.9120(3)	0.3782(2)	0.883	0.018(4)
Cl2	6 <i>c</i>	0.4777(3)	0.9120(3)	0.3782(2)	0.117	0.018(4)
Se3	6 <i>c</i>	0.2537(3)	0.1475(7)	0.1507(3)	0.729	0.032(6)
Cl3	6 <i>c</i>	0.2537(3)	0.1475(7)	0.1507(3)	0.271	0.032(6)

Table S5. Selected bond length for $\text{La}_6\text{Cd}_{0.75}\text{Ga}_2\text{Se}_{11.5}\text{Cl}_{2.5}$

Bond	Bond lengths (Å)	Bond	Bond lengths (Å)
La1-Se1	3.0054	Cd1-Se3	2.6306
La1-Se2	3.0777	Ga1-Se1	2.3663
La1-Se2	3.2457	Ga1-Se2	2.4178
La1-Se2	2.9881	Ga2-Se1	2.394
La1-Se3	2.9970	Ga2-Se2	2.334
La1-Se3	3.0285	Ga2-Se2	2.394
La1-Se3	3.1192	Ga2-Se3	2.423

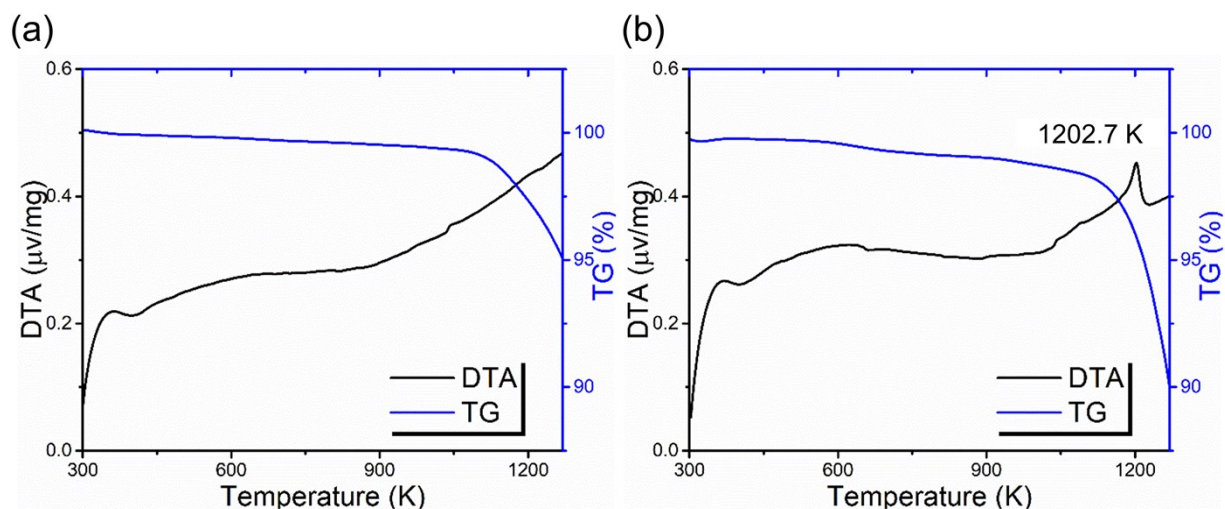


Figure S1. Thermal analysis results for (a) $\text{La}_6\text{Cd}_{0.75}\text{Ga}_2\text{S}_{11.5}\text{Cl}_{2.5}$, and (b) $\text{La}_6\text{Cd}_{0.75}\text{Ga}_2\text{Se}_{11.5}\text{Cl}_{2.5}$

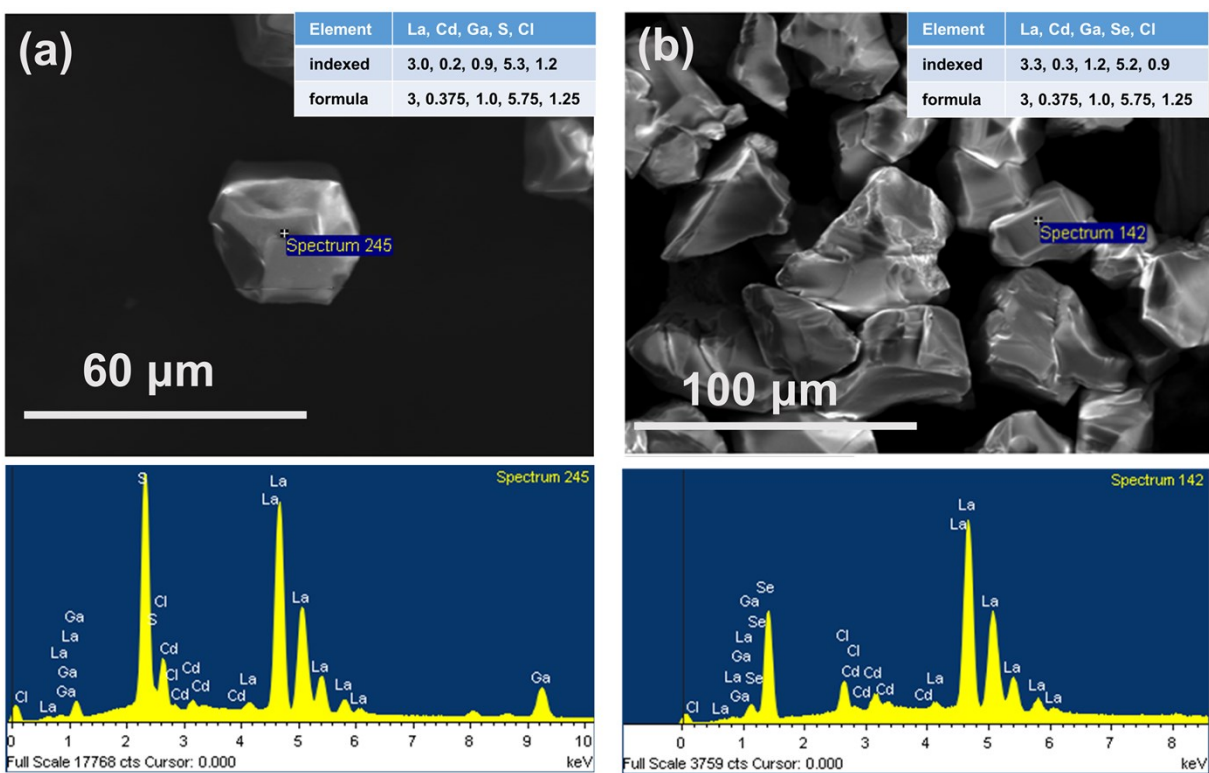


Figure S2. SEM and EDS results for (a) $\text{La}_6\text{Cd}_{0.75}\text{Ga}_2\text{S}_{11.5}\text{Cl}_{2.5}$, and (b) $\text{La}_6\text{Cd}_{0.75}\text{Ga}_2\text{Se}_{11.5}\text{Cl}_{2.5}$

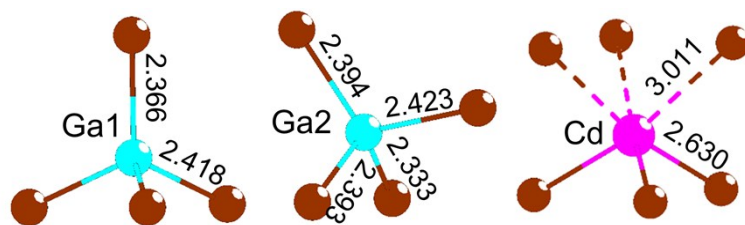


Figure S3. Bond length of each polyhedron in $\text{La}_6\text{Cd}_{0.75}\text{Ga}_2\text{Se}_{11.5}\text{Cl}_{2.5}$